Lecture 16
Convergence and Acceleration of Source Iterations

1 Convergence of Source Iterations

In a previous lecture, it was shown that each source iteration adds the contribution from another generation of scatter to the flux solution. Thus it is clear that the source iteration process will converge quickly whenever particles scatter just a few times on the average before being absorbed or escaping the system. Optically thin or highly absorbing systems clearly fall into this category. It is also clear that the source iteration process will converge very slowly in diffusive problems because the particles can scatter an arbitrary number of times on the average before being absorbed or escaping the system. The purpose of this section is to use Fourier techniques to determine the convergence rate of the source iteration process for a model problem. This model problem is defined by continuum transport rather than the S_n approximation. The scattering is assumed to be isotropic, the transport domain is assumed to be infinite, and the transport medium is characterized by a total cross-section, σ_t, and a scattering cross-section, σ_s. We begin the analysis with the source iteration equations:

$$\mu \frac{\partial \psi^{\ell+1}}{\partial x} + \sigma_t \psi^{\ell+1} = \frac{\sigma_s}{4\pi}\phi^{\ell} + \frac{q_0}{4\pi}\,. \tag{1}$$

where ℓ is the iteration index. The exact transport solution satisfies

$$\mu \frac{\partial \psi}{\partial x} + \sigma_t \psi = \frac{\sigma_s}{4\pi}\phi + \frac{q_0}{4\pi}\,. \tag{2}$$

Subtracting Eq. (1) from Eq. (2), we get an equation that relates the angular flux error at iteration step $\ell + 1$ to the scalar flux error at iteration step ℓ:

$$\mu \frac{\partial \delta\psi^{\ell+1}}{\partial x} + \sigma_t \delta\psi^{\ell+1} = \frac{\sigma_s}{4\pi}\delta\phi^{\ell}\,, \tag{3}$$

where the angular flux error is

$$\delta\psi^{\ell+1} = \psi - \psi^{\ell+1}\,, \tag{4}$$

and the scalar flux error is

$$\delta\phi^{\ell} = \phi - \phi^{\ell} = 2\pi \int_{-1}^{+1} \delta\psi^{\ell}\, d\mu\,. \tag{5}$$

We next make the Fourier anzatz, i.e., we assume that

$$\delta\psi(x,\mu) = \delta\Psi(\lambda,\mu)\exp(i\lambda x)\,, \tag{6}$$

where $i = \sqrt{(}-1)$. The continuum of functions corresponding to $exp(i\lambda x)$ for each value of $\lambda \in (-\infty, +\infty)$ can be used to construct any square-integrable function, $f(x)$. In particular,

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \hat{f}(\lambda)\, \exp(i\lambda x)\, d\lambda\,, \tag{7}$$

where $\hat{f}$ is the Fourier transform of f:

$$\hat{f}(x) = \int_{-\infty}^{+\infty} \hat{f}(x)\, \exp(-i\lambda x)\, dx\,. \tag{8}$$

Thus Eq. (6) is equivalent to assuming that $\delta\psi$ has the spatial dependence of a single continuum basis function. This is particularly useful for two reasons. First, Fourier modes are eigenfunctions of differential spatial operators, making it much easier to invert such operators. Second, if we can determine how the iteration error associated with each mode is attenuated, we can also determine how the iteration errors associated with a general function are attenuated. Substituting from Eq. (6) into into Eq. (3), and dividing the Eq. (3) by $\exp(i\lambda x)$, we get

$$(\mu i\lambda + \sigma_t)\, \delta\Psi^{\ell+1} = \frac{\sigma_s}{4\pi}\delta\Phi^{\ell}\,. \tag{9}$$

Note that the spatial derivative term in Eq. (3) has been replaced with an algebraic expression. Thus we can trivially solve Eq. (9) for $\Psi^{\ell+1}$:

$$\delta\Psi^{\ell+1} = \frac{\sigma_s}{4\pi\,(\mu i\lambda + \sigma_t)}\, \delta\Phi^{\ell}\,. \tag{10}$$

Since we are only iterating on the scalar flux, we need only relate the error in the scalar flux at step $\ell+1$ to the error in the scalar flux at step ℓ. To do this, we simply integrate Eq. (10) over all angles. To facilitate that integration we both divide and multiply the right side of Eq. (10) by the complex conjugate of $\mu i\lambda + \sigma_t$:

$$\delta\Psi^{\ell+1} = \frac{\sigma_s\,(\sigma_t - \mu i\lambda)}{4\pi\,(\mu^2\lambda^2 + \sigma_t^2)}\ \delta\Phi^{\ell}\,. \tag{11}$$

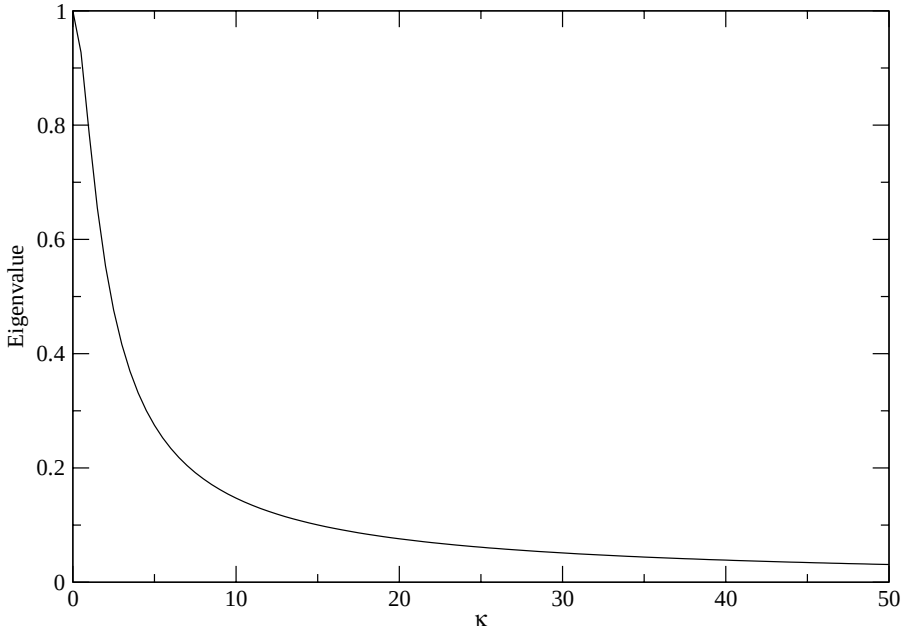

Figure 1: Eigenvalue plot for source iteration with $c = 1$.

the μ-dependent term in the numerator is odd in μ, so

$$\begin{aligned} \delta\Phi^{\ell+1} &= 2\pi \int_{-1}^{+1} \frac{\sigma_s \sigma_t}{4\pi \left(\mu^2 \lambda^2 + \sigma_t^2\right)} \, d\mu \;\; \delta\Phi^{\ell+1} \,, \\ &= \frac{\sigma_s}{\lambda} \arctan\left(\frac{\lambda}{\sigma_t}\right) \;\; \delta\Phi^{\ell} \,. \end{aligned} \tag{12}$$

For plotting purposes, it is useful to re-express Eq. (12) in terms of the scattering ratio, c, and another dimensionless parameter, $\kappa = \lambda/\sigma_t$:

$$\delta\Phi^{\ell+1} = \frac{c}{\kappa} \arctan\left(\kappa\right) \;\; \delta\Phi^{\ell} \,. \tag{13}$$

A plot of this eigenvalue function with $c = 1$ is given in Fig. 1. Because the function is even, we need only consider $\kappa \geq 0$. It can be seen from Fig. 1 that the spectral radius

occurs at $\kappa = 0$ and is equal to the scattering ratio. Thus, the spectral radius is equal to one for a pure scattering medium. Our analysis applies to an infinite medium where no leakage is possible. In real calculations, the spectral radius is not one when $c = 1$, but it can be arbitrarily close to 1. Thus we need to find a way to accelerate the source iteration process when c is close to one.

2 Diffusion-Synthetic Acceleration

One of the most effective ways of accelerating the source iteration process is a technique known as diffusion-synthetic acceleration. The basic idea behind this scheme is first perform a source iteration, and then use a diffusion approximation to estimate the error in the scalar flux iterate. This estimate is then used to improve the accuracy of the iterate. The first step in the derivation of the diffusion-synthetic acceleration scheme is to derive an exact equation for $\delta\psi^{\ell+1}$. We begin this derivation by subtracting the quantity, $\frac{\sigma_s}{4\pi}\,\delta\phi^{\ell+1}$ from both sides of Eq. (3):

$$\mu\,\frac{\partial\delta\psi^{\ell+1}}{\partial x} + \sigma_t\delta\psi^{\ell+1} - \frac{\sigma_s}{4\pi}\delta\phi^{\ell+1} = \frac{\sigma_s}{4\pi}\left(\delta\phi^{\ell} - \delta\phi^{\ell+1}\right)\,. \tag{14}$$

Recognizing that

$$\delta\phi^{\ell} - \delta\phi^{\ell+1} = \left(\phi - \phi^{\ell}\right) - \left(\phi - \phi^{\ell+1}\right) = \phi^{\ell+1} - \phi^{\ell}\,, \tag{15}$$

Eq. (14) can be re-expressed as follows:

$$\mu \frac{\partial \delta\psi^{\ell+1}}{\partial x} + \sigma_t \delta\psi^{\ell+1} - \frac{\sigma_s}{4\pi}\delta\phi^{\ell+1} = \frac{\sigma_s}{4\pi}\left(\phi^{\ell+1} - \phi^{\ell}\right) . \tag{16}$$

Thus we see that the error in the angular flux at iteration step $\ell+1$ satisfies the transport equation with a source equal to

$$R^{\ell+1} = \frac{\sigma_s}{4\pi}\left(\phi^{\ell+1} - \phi^{\ell}\right) . \tag{17}$$

This source represents the residual associated with $\psi^{\ell+1}$. To demonstrate the general nature of the residual, we consider an arbitrary equation of the form,

$$\mathbf{A}x = y\,, \tag{18}$$

where $\mathbf{A}$ is a linear operator, x is the solution, and y is the source. Let $\tilde{x}$ denote any approximation to x. The residual associated with $\tilde{x}$ and Eq. (18) is defined as follows:

$$\tilde{R} = y - \mathbf{A}\tilde{x}\,. \tag{19}$$

If we subtract Eq. (19) from Eq. (18) and algebraically manipulate the result, we find that

$$\mathbf{A}\delta\tilde{x} = \tilde{R}\,, \tag{20}$$

where the error associated with $\tilde{x}$ is denoted by $\delta\tilde{x} = x - \tilde{x}$.

Since Eq. (16) is exact, we can define an iteration process that converges in one accelerated iteration:

$$\mu \frac{\partial \psi^{\ell+\frac{1}{2}}}{\partial x} + \sigma_t \psi^{\ell+\frac{1}{2}} = \frac{\sigma_s}{4\pi}\phi^{\ell} + \frac{q_0}{4\pi}\,. \tag{21a}$$

$$\phi^{\ell+\frac{1}{2}} = 2\pi \int_{-1}^{+1} \psi^{\ell+\frac{1}{2}} \, d\mu \,, \tag{21b}$$

$$\mu \, \frac{\partial \delta\psi^{\ell+\frac{1}{2}}}{\partial x} + \sigma_t \delta\psi^{\ell+\frac{1}{2}} - \frac{\sigma_s}{4\pi} \delta\phi^{\ell+\frac{1}{2}} = \frac{\sigma_s}{4\pi} \left(\phi^{\ell+\frac{1}{2}} - \phi^{\ell} \right) . \tag{21c}$$

$$\phi^{\ell+1} = \phi^{\ell+\frac{1}{2}} + \delta\phi^{\ell+\frac{1}{2}} \,. \tag{21d}$$

However, there is a glaring deficiency in this scheme: the equation for the error is just as hard to solve as the original transport equation itself. The basic theme of all synthetic acceleration schemes is to substitute an approximation to the exact error equation that is simple enough to solve efficiently, but accurate enough to give effective acceleration. In order to see why a diffusion approximation is a good choice, we must consider the nature of the iterative error for those modes that are the most difficult to converge. In particular, we expand Eq. (10) about $\lambda = 0$ to determine the nature of the angular flux error for those modes that are the most difficult to attenuate with a sweep:

$$\delta\Psi^{\ell+1} = \frac{\sigma_s}{4\pi} \left(\frac{1}{\sigma_t} - \mu i \lambda \right) \, \delta\Phi^{\ell} \,. \tag{22}$$

Equation (22) clearly shows that the angular flux error has a linearly anisotropic angular dependence. Since the diffusion approximation is exact for such a dependence, we can expect the diffusion estimate for the scalar flux error to be exact for $\lambda = 0$, thus the accelerated iteration will completely attenuate those errors most poorly attenuated by the sweep. This is good, but it is not the whole story. Since diffusion theory is not exact for the higher frequency modes, we must be concerned that the errors for these modes may

be significantly overestimated, leading to an overall increase in the error for these modes. To determine what actually happens, we first define the diffusion-synthetic acceleration scheme:

$$\mu \frac{\partial \psi^{\ell+\frac{1}{2}}}{\partial x} + \sigma_t \psi^{\ell+\frac{1}{2}} = \frac{\sigma_s}{4\pi}\phi^{\ell} + \frac{q_0}{4\pi}\,. \tag{23a}$$

$$\phi^{\ell+\frac{1}{2}} = 2\pi \int_{-1}^{+1} \psi^{\ell+\frac{1}{2}}\, d\mu\,, \tag{23b}$$

$$-\frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial \Delta\phi^{\ell+\frac{1}{2}}}{\partial x} + \sigma_a \Delta\phi^{\ell+\frac{1}{2}} = \sigma_s\left(\phi^{\ell+\frac{1}{2}} - \phi^{\ell}\right)\,. \tag{23c}$$

$$\phi^{\ell+1} = \phi^{\ell+\frac{1}{2}} + \Delta\phi^{\ell+\frac{1}{2}}\,. \tag{23d}$$

Note that we use $\Delta\phi$ to denote an estimate of the scalar flux error as opposed to $\delta\phi$, which denotes the true error. To analyze the effectiveness of this scheme, we must re-express the DSA algorithm in terms of the error at each step. In particular, we first subtract Eq. (23a) from Eq. (1) to obtain

$$\mu \frac{\partial \delta\psi^{\ell+\frac{1}{2}}}{\partial x} + \sigma_t \delta\psi^{\ell+\frac{1}{2}} = \frac{\sigma_s}{4\pi}\delta\phi^{\ell}\,. \tag{24a}$$

Next we subtract Eq. (23b) from the trivial equation, $\phi = 2\pi \int_{-1}^{+1} \psi^{\ell+\frac{1}{2}}\, d\mu$, to get

$$\delta\phi^{\ell+\frac{1}{2}} = 2\pi \int_{-1}^{+1} \delta\psi^{\ell+\frac{1}{2}}\, d\mu\,. \tag{24b}$$

Next we add the trivial expression, $\sigma_s\,(\phi - \phi)$, to the right side of Eq. (23c) to obtain

$$-\frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial \Delta\phi^{\ell+\frac{1}{2}}}{\partial x} + \sigma_a \Delta\phi^{\ell+\frac{1}{2}} = \sigma_s\left(\delta\phi^{\ell} - \delta\phi^{\ell+\frac{1}{2}}\right)\,. \tag{24c}$$

Finally, we subtract Eq. (23d) from the trivial equation, $\phi = \phi$, to obtain

$$\delta\phi^{\ell+1} = \delta\phi^{\ell+\frac{1}{2}} - \Delta\phi^{\ell+\frac{1}{2}} \,. \tag{24d}$$

We begin a Fourier Fourier analysis of the DSA algorithm, by assuming the Fourier anzatz in Eqs. (24a) through (24d):

$$(\mu i\lambda + \sigma_t)\, \delta\Psi^{\ell+\frac{1}{2}} = \frac{\sigma_s}{4\pi}\delta\Phi^{\ell} \,, \tag{25a}$$

$$\delta\Phi^{\ell+\frac{1}{2}} = 2\pi \int_{-1}^{+1} \delta\Psi^{\ell+\frac{1}{2}}\, d\mu \,, \tag{25b}$$

$$\left(\frac{\lambda^2}{3\sigma_t} + \sigma_a\right) \Delta\Phi^{\ell+\frac{1}{2}} = \sigma_s \left(\delta\Phi^{\ell} - \delta\Phi^{\ell+\frac{1}{2}}\right) \,, \tag{25c}$$

$$\delta\Phi^{\ell+1} = \delta\Phi^{\ell+\frac{1}{2}} - \Delta\Phi^{\ell+\frac{1}{2}} \,. \tag{25d}$$

Solving Eq. (25a) for $\delta\Psi^{\ell+\frac{1}{2}}$ and integrating over all directions, we get

$$\delta\Phi^{\ell+\frac{1}{2}} = \frac{\sigma_s}{\lambda} \arctan\left(\frac{\lambda}{\sigma_t}\right)\, \delta\Phi^{\ell} \,, \tag{26}$$

Substituting from Eq. (26) into the right side of Eq. (25c), and solving for $\Delta\Phi^{\ell+\frac{1}{2}}$, we obtain

$$\Delta\Phi^{\ell+\frac{1}{2}} = \frac{\sigma_s \left[1 - \frac{\sigma_s}{\lambda} \arctan\left(\frac{\lambda}{\sigma_t}\right)\right]}{\frac{\lambda^2}{3\sigma_t} + \sigma_a}\, \delta\Phi^{\ell} \,. \tag{27}$$

Finally, substituting from Eqs. (26) and (27) into Eq. (25d), we obtain an expression that relates the error at step $\ell + 1$ to the error at step ℓ:

$$\delta\Phi^{\ell+1} = \left\{ \frac{\sigma_s}{\lambda} \arctan\left(\frac{\lambda}{\sigma_t}\right) - \frac{\sigma_s \left[1 - \frac{\sigma_s}{\lambda} \arctan\left(\frac{\lambda}{\sigma_t}\right)\right]}{\frac{\lambda^2}{3\sigma_t} + \sigma_a} \right\}\, \delta\Phi^{\ell} \,. \tag{28}$$

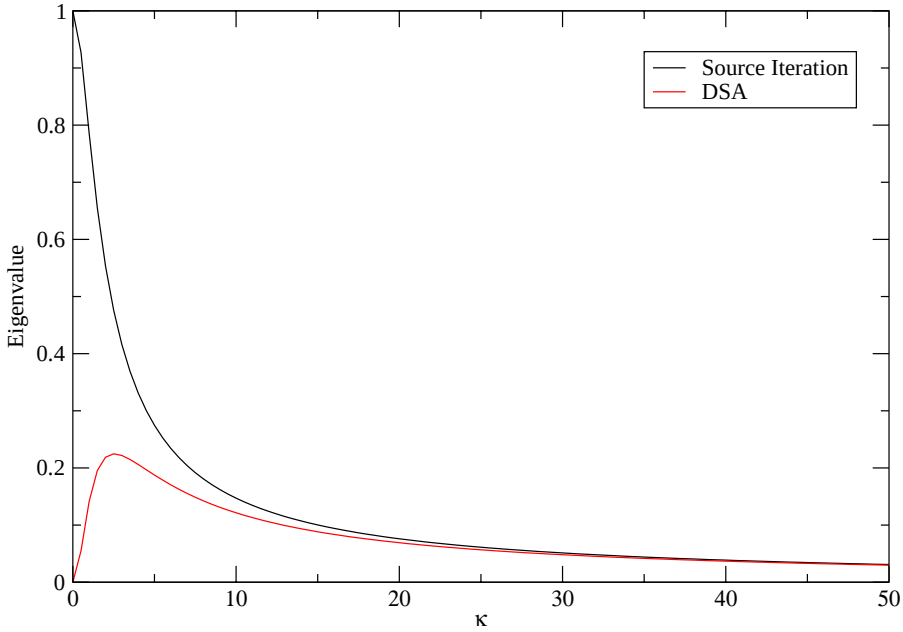

Figure 2: Comparison of source iteration and DSA eigenfunctions with $c = 1$.

for plotting purposes, it is useful to re-express Eq. (28) in terms of the dimensionless parameter, $\kappa = \lambda/\sigma_t$:

$$\delta\Phi^{\ell+1} = \left\{ \frac{c}{\kappa} \arctan(\kappa) - \frac{3c\left[1 - \frac{c}{\kappa}\arctan(\kappa)\right]}{\kappa^2 + 3(1-c)} \right\} \delta\Phi^{\ell} \,. \tag{29}$$

A plot of this eigenfunction together with the source iteration eigenfunction is given in Fig. 2 for $c = 1$. It can be seen from Fig. 2 that the diffusion approximation does indeed annihilate the $\kappa = 0$ error mode, resulting in an accelerated spactral radius equal to reoughly 0.23. For arbitrary c, the spectral radius is roughly $0.23c$. This is an excellent spectral radius. It can also be seen from Fig. 2 that the unaccelerated and accelerated eigenvalues are nearly identical for the high-frequency modes. This means that the diffusion

approximation grossly underestimates the high-frequency errors, which is very good since the source iteration process strongly attenuates them. There is no need for the diffusion to do anything for the high-frequency modes. If the diffusion approximation were to amplify high-frequency modes, the standard method for dealing with it would be to perform more sweeps after the diffusion solve to counter the amplification.

This is standard multigrid strategy. DSA represents a two-grid method because diffusion can be thought of as a "coarse angular grid" approximation to transport. The basic idea of a two-grid methods is to attenuate high-frequency error using a "relaxation scheme", which generally corresponds to some type of local iteration. A coarse-grid operator is then used to estimate the errors with the expectation that the low-frequency errors will be accurately estimated because they can be resolved with a coarse-mesh operator. If the coarse-grid operator amplifies high-frequency errors, more relaxations are added after the coarse-grid correction is made to eliminate the amplification. This is fine as long as the high-frequency errors are not too highly amplified resulting in a requirement for excessive additional relaxations. In a multigrid method, once has a hierachy of grids with each grid estimating the error on the grid above it. This process sounds like it would cost a great deal to execute, but multigrid methods can be very efficient. We can get away with a two-grid method for the transport equation when the scattering is isotropic or linearly anisotropic, but when it is highly anisotropic and forward-peaked, an angular multigrid

method is required. We shall later describe such a method for charged-particle transport calculations.

Provided that the diffusion equation is consistently differenced and the scattering is either isotropic or weakly anisotropic, DSA is an unconditionally effective means of accelerating source iterations. For the most part, this is also true in multidimensional calculations. However, the effectiveness of DSA can be significantly degraded in multidimensional problems with large material discontinuities. However, this deficiency can be overcome by using Krylov methods to solve the S_n equations together with DSA reformulated as a preconditioner. This is a powerful approach. Krylov methods are revolutionizing the way in whch we solve the S_n equations. We will discuss Krylov method in a later lecture.

2.1 Diffusion Boundary Conditions

Our analysis of the DSA method does not require boundary conditions for the diffusion equation because the model problem domain is infinite. However, one must obviously impose boundary conditions on the diffusion equation in real calculations. The principle for deriving diffusion boundary conditions is straightforward. Although we define our DSA algorithm so that the scalar flux is directly updated, one could equivalently update the angular flux as follows:

$$\psi_m^{\ell+1} = \psi_m^{\ell+\frac{1}{2}} + \frac{1}{4\pi}\Delta\phi + \frac{3}{4\pi}\Delta J\mu_m \,, \tag{30}$$

where

$$\Delta J = -\frac{1}{3\sigma_t}\frac{\partial \Delta\phi}{\partial x}\,. \tag{31}$$

Thus we choose the diffusion boundary conditions so that $\psi^{\ell+1}$ satisfies (at least approximately) the correct transport boundary conditions. Equivalently, assume that the error equation is being solved exactly, and choose the transport boundary conditions for that equation so that $\psi^{\ell+1}$ exactly satisfies the correct boundary conditions – then impose these same conditions (at least approximately) on the diffusion solution. As long as the boundary conditions in the S_n calculation are explicit, i.e., met after each source iteration, the boundary conditions for the diffusion equation are simple. In particular, with source or vacuum boundary conditions for the transport solution, the appropriate diffusion boundary condition is vacuum; and with reflective transport boundary conditions, the appropriate diffusion boundary condition is reflective. If the transport boundary condition is reflective and implicit, a boundary source must be added to a reflective diffusion condition to obtain a reflective condition for the hybrid transport/diffusion iterate at step $\ell + 1$. For example, let us assume an implicit reflective transport boundary condition, and let us further assume that the error equation is being solved with the transport equation rather than the diffusion equation. Then the transport iterate at the boundary, $\psi_b^{\ell+\frac{1}{2}}$ will generally not satisfy the reflective condition. We want to choose the conditions for the transport error equation so that the corrected transport iterate will meet the reflective condition. In particular we

want to ensure that

$$\psi^{\ell+\frac{1}{2}}(\mu_m) + \delta\psi^{\ell+\frac{1}{2}}(\mu_m) = \psi^{\ell+\frac{1}{2}}(-\mu_m) + \delta\psi^{\ell+\frac{1}{2}}(-\mu_m)\,, \quad \text{for incoming } \mu_m. \tag{32}$$

Equation (32) can be used to directly define the boundary conditions for the error equation:

$$\delta\psi^{\ell+\frac{1}{2}}(\mu_m) = \psi^{\ell+\frac{1}{2}}(-\mu_m) - \psi^{\ell+\frac{1}{2}}(\mu_m) + \delta\psi^{\ell+\frac{1}{2}}(-\mu_m)\,, \quad \text{for incoming } \mu_m. \tag{33}$$

Equation represents a type of boundary condition known as "reflective plus source," because the incoming flux is equal to the outgoing flux (as in the standard reflective condition) plus a source. The effective source is called the boundary residual:

$$R_b(\mu_m) = \psi^{\ell+\frac{1}{2}}(-\mu_m) - \psi^{\ell+\frac{1}{2}}(\mu_m)\,, \quad \text{for incoming } \mu_m. \tag{34}$$

Note that if the transport iterate meets the reflective boundary condition, the boundary residual is identically zero, and the boundary condition for the error equation is simply reflective. To derive the corresponding boundary condition, we first assume the diffusion dependence of the angular flux in Eq. (33):

$$\frac{1}{4\pi}\Delta\phi^{\ell+\frac{1}{2}} + \frac{3}{4\pi}\Delta J(\mu_m) = R_b(\mu_m) + \frac{1}{4\pi}\Delta\phi^{\ell+\frac{1}{2}} - \frac{3}{4\pi}\Delta J(\mu_m)\,, \quad \text{for incoming } \mu_m. \tag{35}$$

Next, we collect terms in Eq. (35):

$$\frac{3}{2\pi}\Delta J(\mu_m) = R_b(\mu_m)\,, \quad \text{for incoming } \mu_m. \tag{36}$$

Finally, we multiply Eq. (36) by μ_m and integrate over the incoming directions to obtain a fixed current condition:

$$\Delta J = \sum_{\mu_{in}} R_b(\mu_m)\, \mu_m\, w_m\,. \tag{37}$$